

On the Basis of Quantum Statistical Mechanics

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Abstract

We propose a new approach to justify the use of the microcanonical ensemble for isolated macroscopic quantum systems. Since there are huge number of independent observables in a macroscopic system, we cannot see all of them. Actually what we observe can be written in a rather simple combination of local observables. Considering this limitation, we show that almost all states in a energy shell are practically indistinguishable from one another, and hence from the microcanonical ensemble. In particular, the expectation value of a macroscopic observable is very close to its microcanonical ensemble average for almost all states.

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I. INTRODUCTION

Justification of the principles of the equilibrium statistical mechanics is still a controversial problem. For example, the widespread scenario of obtaining the microcanonical ensemble from the ergodicity is not applicable to macroscopic systems, because the "ergodic time" is too long [1].

In this paper we propose an alternative way to justify the use of the microcanonical ensemble for macroscopic quantum systems. The main point is that what we really observe can be written in a rather simple combination of local observables. For example, a macroscopic observable is additive [2], and hence written as a sum of local observables on a proper scale. Therefore we can ignore correlations among macroscopic number of points.

Considering this limitation of observables, we show that almost all pure states in a energy shell look very similar. Therefore we expect that the system go through only typical states with high probability in the course of the time evolution and thus thermal equilibrium is achieved. Note that strong assumptions on the dynamics like ergodicity or mixing are not necessary for a system to reach equilibrium in our picture. It is possible even for an integrable system to reach equilibrium, as has been pointed out in some earlier numerical works [3].

It is known that a typical pure state is highly (almost maximally) entangled in many senses [4]. On the other hand, a thermal state is thought to have no or little amount of entanglement. However, there is no contradiction between the two viewpoints. From our standpoint, a thermal state is a highly entangled state, whose entanglement is too complicated to recognize. In this sense, we can say that too much entanglement is no entanglement.

II. BLOCH VECTOR

To explain the idea more clearly, we introduce the Bloch vector as a tool to represent quantum states. Let \mathcal{H}_N be the Hilbert space of the system whose dimension is N , and V the set of traceless Hermitian operators (i.e., observables) on it. We choose an orthonormal basis set $\{\hat{\lambda}_i | 1 \leq i \leq N^2 - 1\}$ of V . Then the Bloch vector of a state is defined as

$$\boldsymbol{\lambda} \equiv (\langle \hat{\lambda}_1 \rangle, \langle \hat{\lambda}_2 \rangle, \dots, \langle \hat{\lambda}_{N^2-1} \rangle), \quad (1)$$

In this paper, we normalize the basis as

$$\text{Tr}(\hat{\lambda}_i \hat{\lambda}_j) = N \delta_{i,j}, \quad (2)$$

so that the normalization condition for local observables does not depend on the system size. The density matrix $\hat{\rho}$ and the Bloch vector $\boldsymbol{\lambda}$ are related as

$$\hat{\rho} = \frac{1}{N} \left\{ I + \sum_{i=1}^{N^2-1} \langle \hat{\lambda}_i \rangle \hat{\lambda}_i \right\}. \quad (3)$$

We use the L_2 norm for the Bloch vector

$$\|\boldsymbol{\lambda}\| \equiv \sqrt{\sum_i \langle \hat{\lambda}_i \rangle^2} \quad (4)$$

which is related to the Hilbert-Schmidt norm for the density matrix as

$$\|\boldsymbol{\lambda}_A - \boldsymbol{\lambda}_B\| = \sqrt{N \text{Tr}(\hat{\rho}_A - \hat{\rho}_B)^2}. \quad (5)$$

The set of the Bloch vectors is a subset of a ball with radius $\sqrt{N-1}$ in R^{N^2-1} . Pure states are on the surface of the ball, and mixed states are in the interior. At the center, there is the completely mixed state which is represented by the zero-vector $\boldsymbol{\lambda} = 0$.

III. PROJECTION TO THE SPACE OF RELEVANT OBSERVABLES

We consider a macroscopic system composed of n sites, and define a linear subspace of V as

$$V_m \equiv \text{Span} \{ \hat{a}_{\alpha_1}(l_1) \hat{a}_{\alpha_2}(l_2) \dots \hat{a}_{\alpha_k}(l_k) | k \leq m \}. \quad (6)$$

Here, m is a positive integer much smaller than n but still a macroscopic number, and $\{\hat{a}_\alpha(l)\}$ is the basis of local operators at a site l . We normalize the local observables as $\text{Tr}(\hat{a}_\alpha(l) \hat{a}_\beta(l)) = N_s \delta_{\alpha,\beta}$, where N_s is the dimension of the local Hilbert space. V_m contains practically all observables of physical relevance. For example, it contains all macroscopic observables and their low-order moments. We also define a projection operator for the Bloch vector P_{V_m} : $P_{V_m}(\boldsymbol{\lambda})$ is the set of expectation values of all basis elements of V_m .

We pick up a pure state in $\mathcal{H}_{[E, E+\Delta]}$, which is a subspace of the Hilbert space spanned by eigenvectors $|E_i\rangle$ with $E \leq E_i \leq E + \Delta$. A state in $\mathcal{H}_{[E, E+\Delta]}$ is written as

$$|\psi\rangle = \sum_{i \in S} c_i |E_i\rangle, \quad (7)$$

where $S = \{i | E_i \in [E, E + \Delta]\}$. If we choose the coefficients $\{c_i\}$ randomly, the following inequality holds.

$$\overline{\|P_{V_m}(\boldsymbol{\lambda}) - P_{V_m}(\overline{\boldsymbol{\lambda}})\|^2} \leq \frac{N_s^m}{d+1} \dim V_m. \quad (8)$$

Here, $d = \dim \mathcal{H}_{[E, E+\Delta]}$ and the overline represents the ensemble average over all states in $\mathcal{H}_{[E, E+\Delta]}$. With use of Chebyshev's inequality, one can also show

$$\text{Prob}(\|P_{V_m}(\boldsymbol{\lambda}) - P_{V_m}(\overline{\boldsymbol{\lambda}})\| \geq k) \leq \frac{N_s^m \dim V_m}{k^2(d+1)} \quad (9)$$

for any $k > 0$.

As the system size n increases, the density of states increases exponentially but $\dim V_m$ increases only in polynomial order $O(n^m)$. Therefore the RHS of (8) is exponentially small for a macroscopic system, which means that the portion of states practically distinguishable from the microcanonical ensemble is exponentially small.

To prove (8), we first prove the following important lemma

$$\overline{\Delta \langle \hat{\lambda} \rangle^2} \leq \frac{1}{d+1} |\hat{\lambda}|^2, \quad (10)$$

where $\Delta \langle \hat{\lambda} \rangle \equiv \langle \hat{\lambda} \rangle - \overline{\langle \hat{\lambda} \rangle}$ and $|\hat{\lambda}|$ denotes the spectral norm of $\hat{\lambda}$. When we take the ensemble average over $\mathcal{H}_{[E, E+\Delta]}$, $\overline{|c_i|^2} = 1/d$, $\overline{|c_i|^4} = \frac{2}{d(d+1)}$, and $\overline{|c_i|^2 |c_j|^2} = \frac{1}{d(d+1)}$ ($i \neq j$) [4, 5]. Up to the 4-th order, all other combinations vanish identically. Therefore

$$\begin{aligned} & \overline{\Delta \langle \hat{\lambda} \rangle^2} \\ &= \overline{\langle \hat{\lambda} \rangle^2} - \overline{\langle \hat{\lambda} \rangle}^2 \\ &= \sum_{i,j,i',j' \in S} \lambda_{i,j} \lambda_{i',j'} \overline{c_i^* c_j c_{i'}^* c_{j'}} - \left(\sum_{i,j \in S} \lambda_{i,j} \overline{c_i^* c_j} \right)^2 \\ &= \frac{1}{d(d+1)} \sum_{i,j \in S} |\lambda_{i,j}|^2 - \frac{1}{d^2(d+1)} \left(\sum_{i \in S} \lambda_{i,i} \right)^2 \\ &\leq \frac{1}{d(d+1)} \sum_{i,j \in S} |\lambda_{i,j}|^2, \end{aligned} \quad (11)$$

where $\lambda_{i,j} = \langle E_i | \hat{\lambda} | E_j \rangle$. Then

$$\sum_{i,j \in S} |\lambda_{i,j}|^2 \leq \sum_{i \in S} \sum_j |\lambda_{i,j}|^2 \quad (13)$$

$$= \sum_{i \in S} \langle E_i | \hat{\lambda}^2 | E_i \rangle \quad (14)$$

$$= d \overline{\langle \hat{\lambda}^2 \rangle} \quad (15)$$

$$\leq d |\hat{\lambda}|^2. \quad (16)$$

Substituting (16) to (12), we obtain (10). Then, since $|\hat{\lambda}^2| \leq N_s^m$ for any basis element of (6), we obtain (8).

If we consider a small subsystem which consists of less than m sites, all observables in the subsystem is contained in V_m . Since the microcanonical ensemble average of the density matrix of a subsystem is the canonical ensemble in thermodynamically normal systems, (8) gives a justification of the canonical ensemble for a small subsystem.

IV. TIME-DEPENDENT SPIN MODEL

Our idea can be illustrated clearly with a time-dependent spin model. We consider the following Hamiltonian,

$$\begin{aligned}
H = J \sum_{l=1}^N \{ & \sigma_x(l)\sigma_x(l+1) + \sigma_z(l)\sigma_z(l+1) \\
& + \sqrt{2} \cos \phi_l \sigma_y(l)\sigma_y(l+1) \} \\
& - h \sin(\omega t) \sum_{l=1}^N \{ \sin \theta_l \sigma_x(l) + \cos \theta_l \sigma_z(l) \},
\end{aligned} \tag{17}$$

which is a time dependent version of the Hamiltonian used in [4]. Details of this Hamiltonian is not important here. The point is that the time evolution is deterministic and there is no constant of motion in this system.

If we start with a pure state, the state is always pure and the length of the Bloch vector is the maximum value $\sqrt{2^n - 1}$. However, the Bloch vector has so many components that we never see all of them. When we see only small number of components, the Bloch vector looks like the zero-vector with very high probability because the average absolute value of each component is very small. Therefore the system looks like in the completely mixed state, which is the equilibrium state expected from the principle of equal a priori probabilities. Note, however, that the equilibrium is obtained not from any kind of averaging, but from the limitation of observables.

Fig. 1 is the plot of m -body part of the Bloch vector $W_m \equiv \|P_{V_m}(\boldsymbol{\lambda}) - P_{V_{m-1}}(\boldsymbol{\lambda})\|^2$. The initial state is a product state, which has relatively large components for small m . In particular, the one-body part takes the maximum value $W_1 = n$. After some time evolution W_m approaches quickly to the average value $W_m = \frac{3^m n!}{2^n m!(n-m)!}$, which is very small if $m \ll n$. Therefore the system looks like in the completely mixed state.

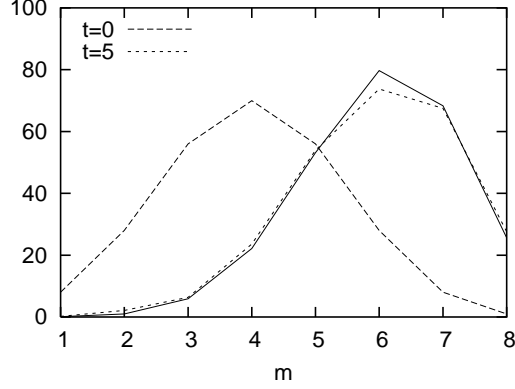


FIG. 1: Plot of W_m for $n = 8$ and $J = h = \omega = 1.0$. The dashed and dotted lines shows the results for $t = 0$ and $t = 5$ respectively. The solid line shows the average over all pure states.

We have also studied the transverse Ising model [3] and confirmed that the system approaches to equilibrium even in the integrable case. Detailed analysis of this model will be reported elsewhere.

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